

Modeling of canine parvovirus NS2 protein

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ABSTRACT

Modeling of canine parvovirus NS2 protein was done using SWISS-MODEL software. Structural details could be elucidated.

Key words: Modeling, CPV, virus, NS1, protein.

INTRODUCTION

Canine parvovirus (CPV) is an important pathogen of dogs and causes serious disease conditions including fatality. The NS2 is a capsid protein. Therefore it is useful to understand the structural details of the vp1 protein.

MATERIALS AND METHODS

Protein

Canine parvovirus isolate Canine/SH/1/2019, complete genome MN840830.1 linear 4269 bp DNA and the amino acid sequence was used for modelling.

Modelling software

<https://swissmodel.expasy.org> was reached to model the protein.

RESULTS AND DISCUSSION

Project summary

MSGNQYTEEVMEGVNWLKKHAENEAFSFVFKCDNVQLNGKDVRWNNYTKP IQNEELTSLIRGAQTAMDQTEEEEMDWESEVDSLAKKL 12
QRLRDASGKQSSSRPSSNSSDSGRSGPCTGT 0

VEYSRYAYCRNCKSTIKPTWRYSQRRASESNVVRNRGRPESHLYF 16
5

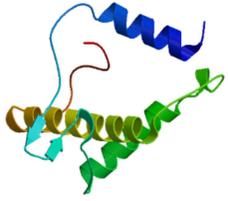
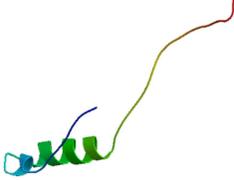
Template Results

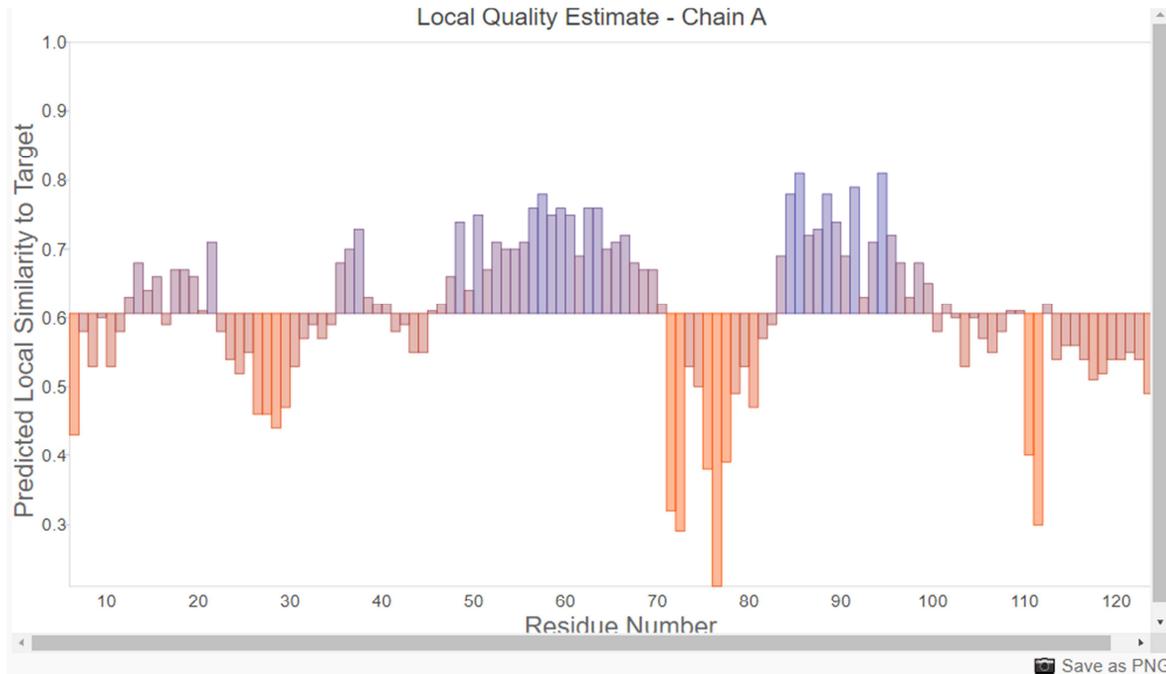
A total of 29 templates were found to match the target sequence. This list was filtered by a heuristic down to 12. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
4r94.1	40.65	monomer	Non-structural protein NS1 Structure of the nickase domain of NS1 from MVM complexed with magnesium
3wrn.1	46.67	monomer	Non-capsid protein NS-1 Minute virus of mice non-structural protein-1N-terminal nuclease domain reveals a unique Zn ²⁺ coordination in the active site pocket and shows a novel mode of

Template	Sequence Identity	Biounit Oligo State	Description
			DNA recognition at the origin of replication
4r94.1	52.08	monomer	Non-structural protein NS1 Structure of the nickase domain of NS1 from MVM complexed with magnesium
3wrn.1	53.26	monomer	Non-capsid protein NS-1 Minute virus of mice non-structural protein-1N-terminal nuclease domain reveals a unique Zn ²⁺ coordination in the active site pocket and shows a novel mode of DNA recognition at the origin of replication
5fil.1	15.56	hetero-22-mer	ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL Bovine mitochondrial ATP synthase state 3b

Model Results

	Id	Template	GMQE	QMEANDisCo	Global	Oligo State	Ligands
	01	4r94.1.A	0.56	0.61 ± 0.08		monomer	-
	02	5fil.1.T	0.11	± 0.12		monomer	-



It is apparent that two models could be constructed and structural details could be elucidated.

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